

METADATA AND NUMERICAL DATA CAPTURE: **Uncertainties** (General Description)

Guided Data Capture (GDC)



This tutorial describes
DATA CAPTURE:
for **Uncertainties** and **Precisions**
with the Guided Data Capture (GDC) software.

NOTE: In GDC 3.0 all *uncertainty* and *precision* information is captured on one form, as shown below. The form appears after the property and metadata (phases, constraints, etc.) are specified.

Uncertainty information

Help

Constraint: Temperature (K)

☐ Uncertainty ← *Most important*

☐ Device specification

☐ Repeatability

Variable 1: Mole fraction of heptane (Dimensionless)

☐ Uncertainty ← *Most important*

☐ Device specification

☐ Repeatability

Property: Vapor or Sublimation pressure (kPa)

☐ Combined uncertainty ← *Most important*

☐ Uncertainty

☐ Device specification

☐ Repeatability

☐ Curve deviation

The **constraints**, **variables**, and **property** shown will correspond to the particular data being captured.

NOTE: Entry of uncertainty information is highly recommended, but *OPTIONAL*.

The most important quantities are the **Uncertainty** (for **constraints** and **variables**) and **Combined Uncertainty** (which is for the **property** only).

The other quantities are measures of **precision** only and represent *lower limits* for the uncertainties.

Definitions follow

Constraint: Temperature (K)

- ☐ Uncertainty  *Most important*
- ☐ Device specification
- ☐ Repeatability

3 General measures of uncertainty/precision are shown for each **constraint, variable, and property**.

The **property** has two additional quantities described later.

You can select to enter any or all of these. Additional fields associated with the quantity appear after selection. (Select by checking the *check box*)

The following pages show each uncertainty/precision type.

Variable 1: Mole fraction of heptane (Dimensionless)

☒ Uncertainty Value: ☐ % Level of confidence: %

☐ Device specification

☐ Repeatability

Uncertainty is the most important quantity for ***variables*** and ***constraints***. This quantity is the ***Expanded Uncertainty*** described in *J. Chem. Eng. Data*, 2003, 48, 1344.

It includes the uncertainty arising from all sources, but *does not include propagation of uncertainty from other constraints or variables*.

The ***value*** for the *entire data set* can be entered as an *absolute value* or *percentage*. (Select the % check box for percentages)

If necessary, *Uncertainties* associated with *individual data points* can be entered in the *Data Table Form* which follows the *Uncertainty Info Form*.

The ***Level of confidence*** is assumed to be **95%**, but you can change this value, if necessary.

Variable 1: Mole fraction of heptane (Dimensionless)

☐ Uncertainty

☒ Device specification Value: ☐ % Level of confidence: % Evaluator:

☐ Repeatability

Device Specification is a type of **precision**.

Device specification allows reporting of *device calibration information*. This does not include uncertainties associated with use of the device in the experimental apparatus.

For example, a thermometer could have a *Device Specification* value of 0.01 K (based on calibration), but the uncertainty in the temperature measurements might be much larger.

The *Device Specification* value is one measure of the **lower limit** for the uncertainty.

The **Level of confidence** is assumed to be **95%**, but you can change this value, if necessary.

Variable 1: Mole fraction of methyl tert-butyl ether (Dimensionless)

☐ Uncertainty

☐ Device specification

☒ Repeatability Value: ☐ % Repetitions:

Repeatability is another type of **precision**.

Repeatability is defined as:

Closeness of the agreement between the results of successive measurements of the same measurand carried out under the **same** conditions of measurement.

Repeatability is expressed in GDC as: the *Standard Deviation of a Single Measurement* or the *Standard Deviation of the Mean*. (Mathematical formulations are given in the HELP file for the **Uncertainty Information** form.

The *Repeatability* value is another measure of the **lower limit** for the uncertainty.

The **Level of confidence** is assumed to be **95%**, but you can change this value, if necessary.

Property: Vapor or Sublimation pressure (kPa)

- ☐ Combined uncertainty
- ☐ Uncertainty
- ☐ Device specification
- ☐ Repeatability
- ☐ Curve deviation

The PROPERTY has 2 additional representations:

- 1) Combined Uncertainty:** This is like the *Uncertainty*, but it includes uncertainty *propagated* from the variables and constraints. This is the most important representation of uncertainty.
- 2) Curve deviation:** This is another measure of the *lower limit* for the uncertainty

Property: Vapor or Sublimation pressure (kPa)

☒ Combined uncertainty Value: ☐ % Level of confidence: %

☐ Uncertainty

☐ Device specification

☐ Repeatability

☐ Curve deviation

The method of determination is selected here.

Propagation of Assessed Std. Deviations
Comparison with Other Measurements

Combined Uncertainty is the most important quantity for properties. This is the *Combined Expanded Uncertainty* described in *J. Chem. Eng. Data*, 2003, 48, 1344.

This quantity includes the uncertainty arising from all sources, *and includes propagation of uncertainty from the constraints or variables.*

The quantity can be entered as an *absolute value* or *percentage*.

You should select how the values were determined from the indicated pull-down menu. (shown in the **red** box above)

The ***Level of confidence*** is assumed to be **95%**, but you can changed this value, if necessary.

Property: Vapor or Sublimation pressure (kPa)

☐ Combined uncertainty

☐ Uncertainty

☐ Device specification

☐ Repeatability

☒ Curve deviation

RMS: ☐ %

Equation type:

The equation type or name can be entered here as text.

Curve deviation is another type of **precision**.

Curve deviation is defined as:

The root-mean-square deviation from a specified curve.

The *Curve deviation* value is another measure of the **lower limit** for the uncertainty.

The value can be expressed as an absolute value or percentage.

The **Level of confidence** is assumed to be **95%**, but you can change this value, if necessary.

Uncertainty information [X]

Help

Constraint: Pressure (kPa)

☒ Uncertainty Value: % Level of confidence: %

☐ Device specification

☐ Repeatability

Variable 1: Temperature (K)

☒ Uncertainty Value: % Level of confidence: %

☐ Device specification

☐ Repeatability

Variable 2: Mole fraction of diethyl carbonate (Dimensionless)

☒ Uncertainty Value: % Level of confidence: %

☐ Device specification

☒ Repeatability Value: % Repetitions:

Property: Viscosity (* 0.001 Pa*s)

☒ Combined uncertainty Value: % ☒ % Level of confidence: %

☐ Uncertainty

☐ Device specification

☐ Repeatability

☐ Curve deviation

OK Cancel

Click **OK**, when the form is complete.

All definitions are based on the following documents:

Definitions and descriptions of all quantities related to the expression of uncertainty in GDC conform to the;

Guide to the Expression of Uncertainty in Measurement, ISO (International Organization for Standardization), October, 1993.

These ISO recommendations were adopted with minor editorial changes as the;

U.S. Guide to the Expression of Uncertainty in Measurement. (commonly referred to by its abbreviation; the *GUM*).

The recommendations have been summarized in;

Guidelines for the Evaluation and Expression of Uncertainty in NIST Measurement Results

This final document is available via free download from the Internet
(<http://physics.nist.gov/cuu/>).

A more complete discussion of the uncertainty terms used here is given in *J. Chem. Eng. Data*, **2003, 48, 1344-1359.**

Note: This article provides much more detail than is necessary for use of GDC.

END

Continue with data capture...